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In the high-density limit the exchange energy easily overcomes the correlation energy in both two- and three-dimensional electron liquids. It is therefore reasonable to inquire if the class of exchange driven instabilities first discussed by Overhauser within the Hartree-Fock theory could be of relevance in this limit. Our analysis shows that this is not the case at least for distorted states represented by a single Slater determinant.

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The high-density limit ground state of an electron liquid has been "known" for quite some time. In this regime, one in which r_s, the average distance between electrons expressed in Bohr radii, is vanishingly small, the kinetic energy dominates and the role of the Coulomb interaction is reasonably expected to be that of a perturbation.[1] Of course that in this limit the electron liquid problem be perturbative in nature is only a very reasonable assumption for, in principle, nothing prevents the electrons to revel in an, to date unknown, exotic broken symmetry ground state.

It is precisely under this perturbative point of view that one is led in the three-dimensional case to the following familiar[1,2] expression for the energy per particle (in Rydbergs):[3]

$$\epsilon_{3D}(r_s) \simeq \frac{2.21}{r_s^2} - \frac{0.916}{r_s} + 0.062 \ln r_s - 0.093 + \mathcal{O}(r_s \ln r_s), \tag{1}$$

where the jellium model of the electron liquid has been assumed for simplicity. In the two-dimensional case a similar expression applies:[4,5]

$$\epsilon_{2D}(r_s) \simeq \frac{1}{r_s^2} - \frac{1.2}{r_s} - (0.38 \pm 0.04) - 0.17 r_s \ln r_s + \mathcal{O}(r_s). \tag{2}$$

As one would expect, the kinetic aspects of the problem becoming increasingly important, it is the exchange energy, with its kinematic origin, that dominates the Coulomb interaction contributions: The correlation energy becomes seemingly irrelevant for $r_s \to 0$. It is therefore reasonable to entertain the notion that the type of exchange driven instability of the homogeneous paramagnetic state discovered by A. W. Overhauser[6] be relevant in this regime.

As Overhauser showed, if correlation effects are neglected (i.e., if the wave function is taken to be a simple Slater determinant of one-electron orbitals), it is always possible to lower the energy of an otherwise homogeneous, paramagnetic electronic liquid, by introducing in it certain spin- and charge-density-wave-type distortions.[6,7] This mechanism results in corresponding spin-density wave (SDW), charge-density wave (CDW) and mixed CDW-SDW states.[8] What is rather remarkable is that Overhauser's instability theorem, while crucially depending on the long range of the Coulomb interaction, is valid for all densities. This suggests that, by going to sufficiently high density, one might enter a regime in which the correlation energy becomes irrelevant and therefore is no longer able to preempt the exchange driven instability. In particular one may wonder if a single Slater determinant with SDW character might have lower energy than the fully correlated homogeneous ground state. For this to happen, however, it is not sufficient that the correlation energy be much smaller than the exchange energy. A much stronger condition must be satisfied, namely that the correlation energy[9,10] be smaller than the exchange energy *gained* in an SDW or CDW distorted single Slater determinant. We will show that this is not the case. The exchange energy gained by going from the homogeneous Slater determinant to a Slater determinant with SDW character is exponentially small at high density, and is therefore totally swamped by the correlation energy of the homogeneous Fermi liquid ground state.

We begin by discussing some of the crucial details of the Overhauser's instability theorem at zero temperature. Although perhaps less pictorial than the original, we find more straightforward and accessible to proceed with an algebraic version of the proof. The latter involves employing the density matrix operator whose matrix elements in the plane waves representation are defined by $\rho_{\vec{k}\sigma,\vec{p}\mu} = \langle \hat{a}^\dagger_{\vec{k}\sigma} \hat{a}_{\vec{p}\mu} \rangle$. For example a single Slater determinantal paramagnetic state made out of plane waves can be represented by the following density matrix:

$$\rho^{(0)}_{\vec{k}\sigma,\vec{p}\mu} = n_{\vec{k}\sigma} \delta_{\vec{k},\vec{p}} \delta_{\sigma,\mu}. \tag{3}$$

We then postulate a single Slater determinant state constructed by occupying not plane waves but rather the distorted wave functions,

$$\phi_{\vec{k}}(\vec{r},\sigma) \propto e^{i\vec{k}\cdot\vec{r}} + A_{\vec{k}+\vec{Q},\vec{k},\sigma} e^{i(\vec{k}+\vec{Q})\cdot\vec{r}} + A_{\vec{k}-\vec{Q},\vec{k},\sigma} e^{i(\vec{k}-\vec{Q})\cdot\vec{r}}. \tag{4}$$

This corresponds to a SDW, a CDW or a mixed state depending on the choice of the distortion amplitudes A's. Notice that this state does not represent a self-consistent solution of the Hartree-Fock equations and should be only taken as a suitable variational state.

The corresponding modified density matrix is readily seen to be given by

$$\rho_{\vec{k}\sigma,\vec{p}\mu} = \rho^{(0)}_{\vec{k}\sigma,\vec{p}\mu} + \delta\rho_{\vec{k}\sigma,\vec{p}\mu}, \tag{5}$$

where the correction $\delta\rho_{\vec{k}\sigma,\vec{p}\mu}$ can be inferred from the form of Eq. (4).

Then, if one makes the educated choice $\vec{Q}=2k_F\hat{n}$, with $\hat{n}$ an arbitrary unit vector in two or three dimensions, the condition $|\vec{k}\pm\vec{Q}|>k_F$ is automatically satisfied when $k<k_F$ and the only nonvanishing matrix elements of $\delta\rho$ have the form

$$\begin{aligned}\delta\rho_{\vec{k}+\vec{Q}/2\sigma,\vec{k}-\vec{Q}/2\sigma} &= \delta\rho_{\vec{k}-\vec{Q}/2\sigma,\vec{k}+\vec{Q}/2\sigma} \\ &= (n_{\vec{k}+\vec{Q}/2} + n_{\vec{k}-\vec{Q}/2})A_{\vec{k}+\vec{Q}/2,\vec{k}-\vec{Q}/2,\sigma}.\end{aligned} \tag{6}$$

At this point we simply introduce a variational Ansatz for the amplitudes, i.e., choose

$$A_{\vec{k}+\vec{Q}/2,\vec{k}-\vec{Q}/2,\uparrow} = \begin{cases} \dfrac{(bk_F)^2}{\ln^2 b}\left|\dfrac{n_{\vec{k}+\vec{Q}/2}-n_{\vec{k}-\vec{Q}/2}}{k^2\cos\theta}\right| & bk_F<k<bek_F, \\ 0 & \text{otherwise}, \end{cases} \tag{7}$$

where θ is the angle between $\vec{k}$ and $\vec{Q}$, and b is a sufficiently small arbitrary positive variational parameter. Moreover for the sake of argument we take $A_{\vec{k}+\vec{Q}/2,\vec{k}-\vec{Q}/2,\downarrow}=-A_{\vec{k}+\vec{Q}/2,\vec{k}-\vec{Q}/2,\uparrow}$, which is the case of a linear spin-density wave.

At this point the change in energy ΔE associated with the distortion can be readily evaluated to lowest order in the amplitudes by means of the general formula involving the corrections to the density matrix:

$$\begin{aligned}\Delta^{(2)}E_{HF} = &\frac{1}{2}\sum_{(\vec{k}\sigma,\vec{p}\tau)}\frac{\varepsilon_{\vec{p}}-\varepsilon_{\vec{k}}}{n_{\vec{k}}-n_{\vec{p}}}\delta\rho_{\vec{k}\sigma,\vec{p}\tau}\delta\rho_{\vec{p}\tau,\vec{k}\sigma} \\ &+\frac{1}{2}\sum_{(\vec{k}\sigma,\vec{k}'\sigma')}\sum_{(\vec{p}\tau,\vec{p}'\tau')}(v_{\vec{k}\sigma\vec{p}\tau\vec{p}'\tau'\vec{k}'\sigma'} \\ &-v_{\vec{k}\sigma\vec{p}\tau\vec{k}'\sigma'\vec{p}'\tau'})\delta\rho_{\vec{k}\sigma,\vec{k}'\sigma'}\delta\rho_{\vec{p}\tau,\vec{p}'\tau'},\end{aligned} \tag{8}$$

where $\varepsilon_{\vec{k}}$ are the Hartree-Fock eigenvalues in the uniform paramagnetic phase.

A direct inspection of the expression obtained by substituting the explicit formula of Eq. (7) into Eq. (8) leads to the following result:

$$\Delta^{(2)}E_{HF} \simeq \frac{\alpha}{r_s}b^4 - \frac{\beta}{r_s}b^4|\ln b| + \frac{\gamma}{r_s^2}\frac{b^4}{|\ln b|}, \tag{9}$$

where it suffices to know that α, β and γ are all positive. In this expression the second term comes from the exchange while the third one is due to the kinetic energy. The first term is best described as an interaction contribution to the kinetic energy. It is important to realize that the structure of this formula (in particular, the $|\ln b|$ in the second term) is a direct consequence of the long range of the Coulomb interaction: The use of a screened interaction would qualitatively spoil the analysis.

Equation (9) shows that, if the correlation energy is for a moment neglected (i.e., within Hartree-Fock), for a given r_s one can always construct a distorted state of lower energy. For the exchange signature term, the second one, can always be made to overcome the first one for sufficiently small values of the variational parameter b. This suffices to establish Overhauser's instability theorem in both two and three dimensions.

Consider next the situation in the high-density limit. In this case it is the third, and usually neglected contribution in Eq. (9) that is of relevance since in this case it forces the value of b to be of order

$$b \approx e^{-\sqrt{\frac{\gamma}{\beta r_s}}}. \tag{10}$$

This leads to an energy gain associated with the distortion of order $e^{-\sqrt{16\frac{\gamma}{\beta r_s}}}/r_s^{3/2}$, something that is easily defeated even by the vanishingly small correlation energy contributions of Eqs. (1) and (2).

The overall picture is then clear. Although in the high-density limit the exchange energy is much larger than the correlation energy, the kinetic energy is even larger than the exchange energy and endeavors to keep the system uniform. In order to avoid the kinetic energy cost, the SDW deformation must be restricted to an infinitesimally small region of the Fermi surface (exponentially vanishing b). But then, at least for a single Slater determinant SDW state, the energy gain is also vanishingly small, and cannot compete with the correlation energy of the uniform state.

This picture does not depend on the specific form of the deformation chosen in Eq. (7). Any deformation that is soft enough to allow the exchange energy to prevail on the kinetic energy, will be far too small to lower the energy below that of the exact homogeneous ground state.

Thus, the main tenet of the Fermi liquid theory—the stability of the homogeneous phase at sufficiently high density—is, within the present study, fully vindicated. It must however be noted that the statement cannot be generalized to include all distorted states since, even at high density, to date it has not been possible to write down and obtain the energy of a fully correlated SDW or CDW distorted state.

We note in closing that the analysis presented in this paper, including a proof of Overhauser's instability theorem, has recently been extended to the case of a two-dimensional electron gas with linear Rashba spin-orbit coupling.[11]

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